AMENDMENT TO THE CLAIMS

1. (*Currently amended*) A program storage device accessible by a computer, tangible embodying a program of instructions executable by said computer to perform method steps for protein structure alignment, ~~said methods steps~~ comprising ~~of~~:

(a) <u>means for</u> receiving <u>atomic coordinates of</u> a first protein with N_1 atoms;

(b) <u>means for</u> receiving <u>atomic coordinates of</u> a second protein with N_2 atoms;

(c) <u>means for</u> making an initial alignment of said atoms of said first protein to said atoms of said second protein;

(d) <u>means for</u> calculating all atomic distances between said <u>atomic</u> coordinates of said atoms of said first protein and said atomic coordinates of said atoms of said second protein;

(e) <u>means for</u> defining a matrix with a plurality of binary assignment variables wherein each binary assignment variable corresponding to either a match or to a gap;

(f) <u>means for</u> defining one or more mean field equations wherein said plurality of binary assignment variables are replaced by a plurality of continuous mean field variables, whereby said each mean field variable has a value between 0 and 1, and a plurality of forces that are proportional to said atomic distances squared;

(g) <u>means for</u> formulating an energy function, wherein:

said energy function includes a first cost for each said atomic distance wherein said distance is a weighted body transformation using said continuous mean field variables of said first protein while keeping said second protein fixed~~;~~ <u>,</u>

said energy function includes a second cost λ for each said gap by either said first protein or said second protein,

said energy function includes a third cost δ for a position-independent consecutive said gap~~;~~ <u>,</u>

said energy function includes a fourth cost for enforcing a constraint to satisfy that each said atom of said first protein either aligns with said atom of said second protein or to said gap;

(h) <u>means for</u> minimizing by an iterative process of said energy function and updating said continuous mean field variables in said mean field equations for a decreasing set of temperatures T until convergence to a predefined convergence value is reached; and

(i) <u>means for</u> after convergence rounding off said continuous mean field variables to either 0 or 1.

2. (*Currently amended*) The <u>program storage device</u> ~~method~~ as set forth in claim 1, wherein said <u>means for</u> ~~step of~~ formulating an energy function further comprises a fifth cost for discouraging crossed matches.

3. (*Currently amended*) The <u>program storage device</u> ~~method~~ as set forth in claim 1, wherein said second cost λ is a value between 0.01 and 0.5.

4. (*Currently amended*) The <u>program storage device</u> ~~method~~ as set forth in claim 3, wherein said second cost λ for a α-site in a α-helix has a larger said second cost λ by a factor between 0.01 and 0.5 of said second cost λ.

5. (*Currently amended*) The <u>program storage device</u> ~~method~~ as set forth in claim 3, wherein said second cost λ for a β-sheet has a larger said second cost λ by a factor between 0.01 and 0.5 of said second cost λ.

6. (*Currently amended*) The <u>program storage device</u> ~~method~~ as set forth in claim 1, wherein said third cost δ is a function of said second cost λ divided by a value between 1 and 20.

7. (*Currently amended*) The program storage device ~~method~~ as set forth in claim 1, wherein fourth cost includes a parameter γ with a value between 0 and 0.2.

8. (*Currently amended*) The program storage device ~~method~~ as set forth in claim 1, wherein said means for ~~step of~~ minimizing by an iterative process includes an iteration parameter ε with a value between 0.5 and 0.95.

9. (*Currently amended*) The program storage device ~~method~~ as set forth in claim 1, wherein said means for ~~step of~~ minimizing by an iterative process further comprises the step of initiating said temperature to a value between 1 and 100.

10. (*Currently amended*) A method of using a mean field approach for protein structure alignment, comprising the steps of:

(a) ~~providing~~ receiving atomic coordinates of a first protein with N_1 atoms;

(b) ~~providing~~ receiving atomic coordinates of a second protein with N_2 atoms;

(c) making an initial alignment of said atoms of said first protein to said atoms of said second protein;

(d) calculating all atomic distances between said atomic coordinates of said atoms of said first protein and said atomic coordinates of said atoms of said second protein;

(e) defining a matrix with a plurality of binary assignment variables wherein each binary assignment variable corresponding to either a match or to a gap;

(f) defining one or more mean field equations wherein said plurality of binary assignment variables are replaced by a plurality of continuous mean field variables, whereby said each mean field variable has a value between 0 and 1, and a plurality of forces that are proportional to said atomic distances squared;

(g) formulating an energy function, wherein:

said energy function includes a first cost for each said atomic distance wherein said distance is a weighted body transformation using said continuous mean field variables of said first protein while keeping said second protein fixed~~;~~,

said energy function includes a second cost λ for each said gap by either said first protein or said second protein,

said energy function includes a third cost δ for a position-independent consecutive said gap~~;~~,

said energy function includes a fourth cost for enforcing a constraint to satisfy that each said atom of said first protein either aligns with said atom of said second protein or to said gap;

(h) minimizing by an iterative process of said energy function and updating said continuous mean field variables in said mean field equations for a decreasing set of temperatures T until convergence to a predefined convergence value is reached; and

(i) after convergence rounding off said continuous mean field variables to either 0 or 1.

11. (*Original*) The method as set forth in claim 10, wherein said step of formulating an energy function further comprises a fifth cost for discouraging crossed matches.

12. (*Original*) The method as set forth in claim 10, wherein said second cost λ is a value between 0.01 and 0.5.

13. (*Original*) The method as set forth in claim 12, wherein said second cost λ for a α-site in a α-helix has a larger said second cost λ by a factor between 0.01 and 0.5 of said second cost λ.

14. (*Original*) The method as set forth in claim 12, wherein said second cost λ for a β-sheet has a larger said second cost λ by a factor between 0.01 and 0.5 of said second cost λ.

15. (*Original*) The method as set forth in claim 10, wherein said third cost δ is a function of said second cost λ divided by a value between 1 and 20.

16. (*Original*) The method as set forth in claim 10, wherein fourth cost includes a parameter γ with a value between 0 and 0.2.

17. (*Original*) The method as set forth in claim 10, wherein said step of minimizing by an iterative process includes an iteration parameter ε with a value between 0.5 and 0.95.

18. (*Original*) The method as set forth in claim 10, wherein said step of minimizing by an iterative process further comprises the step of initiating said temperature to a value between 1 and 100.